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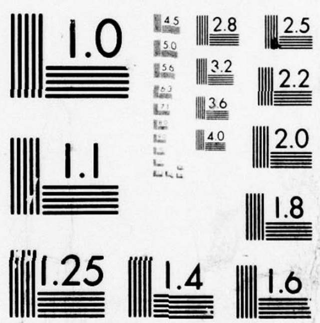

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SOME PROPERTIES OF BEST LINEAR UNBIASED PREDICTORS AND RELATED PREDICTORS

by

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ABSTRACT

The variation of temperature or of pollutant concentrations over a geographic area are adequately represented by random fields. Given a real-valued random field $\{Z(x), x \in \mathbb{R}^2\}$ a basic problem is to interpolate Z over an area A from measurements taken at n stations $x_1, x_2, \ldots, x_n$, when the distribution of Z is only partially specified. This is the motivation of the present paper.

It is shown that if the joint distributions are Gaussian the best linear unbiased predictor is (among other properties) admissible when used to predict Z at a single point, but inadmissible in general when used to predict the values of the field at several points. A Stein-like predictor is produced which is uniformly better than the B.L.U.E. in the latter case. A nonlinear predictor, based on relaxing the unbiasedness condition on the B.L.U.E., is also proposed and shown to be in some cases preferable.

Key words: Best linear unbiased predictor, multivariate normal distribution, admissibility, James-Stein estimation.

1. Introduction and summary:

The questions considered in this paper arise naturally when trying to interpolate a realization of a random field $\{Z(x), x \in \mathbb{R}^2\}$ from observations $Z(x_1), Z(x_2), \ldots, Z(x_n)$ made at n points, for example interpolation of air pollutant concentration field from fixed monitoring stations. The first step is to study how to interpolate at a single point x ; and then, to study how to interpolate simultaneously at N points forming a fine grid, say, over an area of interest.

However in the present paper we study the abstract prediction problem, independently of the geometry of the underlying set of the random field. So consider $n+1$ real valued random variables $Z_1, Z_2, \ldots Z_n$ and Z with a joint distribution whose covariance matrix is specified and whose mean vector is the product of a specified matrix by an unspecified p-dimensional vector parameter a.

First of all, in Section 2, we are interested in the properties of the best linear unbiased predictor $\hat{Z}$ of Z based on the observed values of $Z_1, Z_2, \ldots, Z_n$, when the risk function is $R(a,\hat{Z}) = E(\hat{Z}-Z)^2$. We show that if the joint distribution of $Z_1, Z_2, \ldots, Z_n$ and Z is normal, then $\hat{Z}$ is extended Bayes, minimax, admissible and uniformly minimum variance unbiased.

Then in Section 3 we consider the problem of predicting

simultaneously N random variables $Z_{n+1}, Z_{n+2}, \ldots, Z_{n+N}$ (instead of a single Z) on the basis of the observed values of $Z_1, Z_2, \ldots, Z_n$. Under the risk function

$$\sum_{i=1}^{N} E(\hat{Z}_{n+i} - Z_{n+i})^2$$

we show that the pointwise use of the best linear unbiased predictor of Section 2 for each Z_i, $i = n+1,\ldots,n+N$ is not an admissible procedure in general under normality assumption. This is done by constructing a Stein-like predictor $(\tilde{Z}_{n+1}, \tilde{Z}_{n+2}, \ldots, \tilde{Z}_{n+N})$ for $(Z_{n+1}, Z_{n+2}, \ldots, Z_{n+N})$. A necessary and sufficient condition for the Stein-like predictor to be uniformly better than the simultaneous pointwise best linear unbiased predictor $(\hat{Z}_{n+1}, \hat{Z}_{n+2}, \hat{Z}_{n+N})$ is given. It is derived as a consequence of the following result (proved in Section 3): If X is a p-dimensional normal random vector with distribution $N(\theta, I_p)$ and C is a fixed $N \times p$ matrix then $\exists \eta > 0$ such that $\forall \theta$

$$(1) \qquad E\left\| CX\left(1 - \frac{\eta}{\|X\|^2}\right) - C\theta \right\|^2 < E\|CX - C\theta\|^2$$

if and only if

$$(2) \qquad \text{max eigenvalue of } CC' < \tfrac{1}{2}\, \mathrm{tr}\, CC'$$

This theorem extends the basic result of James and Stein (1961) which says that in the case $C = I_p$ the N.S.C. for (1) to hold is $p \geq 3$.

Finally, in Section 4, going back to the problem of predicting a single Z , we present a biased non-linear predictor Z^* obtained as a modification of $\hat{Z}$ when the unbiasedness condition is relaxed. We compute the risk function of Z^* and conclude that Z^* should be preferred to $\hat{Z}$ in some cases when the unspecified vector parameter a can be bounded.

2. The best linear unbiased predictor of a single random variable and its properties in the normal case:

Preliminaries:

Let $\underline{Z}$ denote the column vector formed by the observed values $(Z_1, Z_2, \ldots, Z_n)$. Then the assumptions described in Section 1 can be written as follows:

$$E\,\underline{Z} = F'a \quad , \quad \text{Cov}\,\underline{Z} = K$$

$$E\,Z = f'a \quad , \quad \text{var}\,Z = \sigma^2$$

$$\text{Cov}(\underline{Z}, Z) = k$$

F ($p\times n$ matrix), f ($p\times 1$), K ($n\times n$), k ($n\times 1$) ,

and σ^2 (scalar) are specified quantities.

a ($p\times 1$ vector) is an unspecified vector-parameter.

The best linear unbiased predictor $\hat{Z} = \lambda_o + \lambda_1 Z_1 + \lambda_2 Z_2 + \ldots + \lambda_n Z_n$ (that we write in short $\hat{Z} = \lambda_o + \lambda'\underline{Z}$) of Z is obtained by solving the following system

$$\begin{cases} E(\hat{Z}-Z)^2 \text{ minimum} & 2.1.a \\ E\,\hat{Z} = f'a \text{ for all } a & 2.1.b \end{cases}$$

The minimization, in 2.1.a , a priori depends on a , but

condition 2.1.b. implies $\lambda_o = 0$, $F\lambda = f$, and $E(\hat{Z}-Z)^2$ independent of a. The solution, which is classical, is

$$\lambda = K^{-1}k - K^{-1}F'(FK^{-1}F')^{-1}FK^{-1}k + K^{-1}F'(FK^{-1}F')^{-1}f \qquad 2.2$$

and the mean square error of the best $\hat{Z}$ is

$$E(\hat{Z}-Z)^2 = \mathrm{Var}(\hat{Z}-Z) =$$
$$\sigma^2 - k'K^{-1}k + (FK^{-1}k - f)'(FK^{-1}F')^{-1}(FK^{-1}k - f) \qquad 2.3$$

For subsequent use of these unwieldy formulas we introduce the following notation: $G = FK^{-1}F'$ (we assume it is non singular), and $\Phi = FK^{-1}k - f$.

$\hat{Z}$ can be given a simple interpretation (Goldberger, 1962): since $\underline{Z} = F'a + \varepsilon$ where $E\varepsilon = 0$ and $\mathrm{Cov}\ \varepsilon = K$. The generalized least square estimator of a based on $\underline{Z}$ is $\hat{a} = (FK^{-1}F')^{-1}FK^{-1}\underline{Z} = G^{-1}FK^{-1}\underline{Z}$ and the best linear unbiased predictor of Z can be rewritten

$$\hat{Z} = f'\hat{a} + k'K^{-1}[\underline{Z}-F'\hat{a}] \qquad 2.4$$

Formula 2.4, in view of the best linear predictor

$$\hat{Z} = f'a + k'K^{-1}[\underline{Z}-F'a] \qquad 2.5$$

of Z when a is specified, shows the natural origin of $\hat{Z}$.

Finally let us observe that $E(\hat{Z}-Z)^2 = \sigma^2 - k'K^{-1}k + \emptyset'G^{-1}\emptyset$ and $E(\tilde{Z}-Z)^2 = \sigma^2 - k'K^{-1}k$. Therefore $\emptyset'G^{-1}\emptyset$ represents the price we pay for not knowing a, while requiring unbiasedness of $\hat{Z}$. In Section 3 and Section 4 we show how this added term in the mean square error may be reduced.

<u>Properties of $\hat{Z}$ in the normal case:</u>

In addition to the assumptions laid out at the beginning of this Section, we now assume that Z and $\underline{Z}$ are jointly multivariate normal.

First of all suppose that the vector parameter a has the multivariate normal prior distribution $N(\alpha,\Gamma)$

<u>Lemma 2.1:</u> Let $\hat{Z}_{\alpha,\Gamma}$ be the Bayes rule using mean squared error to predict Z, when we observe $\underline{Z}$, and when $a \sim N(\alpha,\Gamma)$. It has the form

$$\hat{Z}_{\alpha,\Gamma} = k'K^{-1}\underline{Z} - \emptyset'E(a|\underline{Z}) \qquad 2.6$$

and its Bayes risk is

$$r(\hat{Z}_{\alpha,\Gamma}) = \sigma^2 - k'K^{-1}k + \emptyset'(G+\Gamma^{-1})^{-1}G(G+\Gamma^{-1})^{-1}\emptyset \qquad 2.7$$

<u>Proof:</u> The Bayes rule $\hat{Z}_{\alpha,\Gamma}$ is the mean of the posterior distribution of Z given $\underline{Z}$, after averaging of over a

$$\begin{aligned}\hat{Z}_{\alpha,\Gamma} &= E\{E(Z|\underline{Z},a)|\underline{Z}\} \\ &= f'E(a|\underline{Z}) + k'K^{-1}\{\underline{Z} - F'E(a|\underline{Z})\} \\ &= k'K^{-1}\underline{Z} - \emptyset'E(a|\underline{Z})\end{aligned}$$

This establishes formula 2.6. The proof of formula 2.7 is omitted because the calculations are straightforward and tedious, using the fact that $E(a|\underline{Z}) = (G+\Gamma^{-1})^{-1}\Gamma^{-1}\alpha + (G+\Gamma^{-1})^{-1}FK^{-1}\underline{Z}$

<u>Theorem 2.1:</u> The best linear unbiased predictor $\hat{Z}$ of Z is extended Bayes and minimax.

<u>Proof:</u> The risk of $\hat{Z}$ as a function of a is $R(a,\hat{Z}) = \alpha^2 - k'K^{-1}k + \emptyset'G^{-1}\emptyset$. This expression does not depend on a, therefore $\hat{Z}$ is an equalizer. Secondly, when all the eigen values of Γ tend to $+\infty$, the risk of $\hat{Z}_{\alpha,\Gamma}$, given by 2.7, tends to $R(a,\hat{Z})$. Therefore $\hat{Z}$ is extended Bayes, and since it is an equalizer it must be minimax. ■

The next two problems are to show that $\hat{Z}$ is admissible and UMVUE. So now we abandon the assumption that a has a prior distribution and return to the case when it is a free unspecified vector-parameter.

<u>Lemma 2.2:</u> For any predictor Z^* of Z based on $\underline{Z}$ we have

$$E(Z^*-Z)^2 = \sigma^2 - k'K^{-1}k + E\{Z^*-E(Z|\underline{Z})\}^2 \qquad 2.8$$

<u>Proof:</u> $Z - Z^*$ can be written as the sum of $Z - E(Z|\underline{Z})$ and $E(Z|\underline{Z}) - Z^*$. Next, $Z - E(Z|\underline{Z})$ is uncorrelated with $\underline{Z}$;

hence, by normality it is independent of $\underline{Z}$, and independent also of $E(Z|\underline{Z}) - Z^*$ because this is a function of $\underline{Z}$. Formula 2.8 follows. ■

<u>Lemma 2.3:</u> $\hat{a} = G^{-1}FK^{-1}\underline{Z}$ is a sufficient estimator for a , among the estimators based on $\underline{Z}$.

This is a standard result in generalized regression. We may just mention for completeness that $E(\underline{Z}|\hat{a}) = F'\hat{a}$ and $\text{Cov}(\underline{Z}|\hat{a}) = K - F'G^{-1}F$. Hence $\underline{Z}$ given $\hat{a}$, which is normally distributed, has a distribution which does not depend on a .

<u>Theorem 2.2:</u> $\hat{Z}$ is an admissible predictor of Z.

<u>Proof:</u> Suppose that $\hat{Z}$ is not admissible and that $Z^* = g(\underline{Z})$ is such that

$$E(Z^*-Z)^2 \leq E(\hat{Z}-Z)^2 \qquad 2.9$$

for all a with strict inequality for at least one a . Then from lemma 2.2 we deduce that

$$E\{Z^*-E(Z|\underline{Z})\}^2 \leq E\{\hat{Z}-E(Z|\underline{Z})\}^2 \qquad 2.10$$

for all a , with strict inequality for at least one a.

$$E(Z|\underline{Z}) = k'K^{-1}\underline{Z} - \emptyset'a \quad \text{, and}$$
$$\hat{Z} = k'K^{-1}\underline{Z} - \emptyset'\hat{a}$$

Therefore, pursuing our argument, we have

$$E\{k'K^{-1}\underline{Z}-g(\underline{Z})-\emptyset'a\}^2 \leq E\{\emptyset'\hat{a}-\emptyset'a\}^2 \qquad 2.11$$

for all a, with strict inequality for at least one a.

Then by lemma 2.3 and the Rao-Blackwell theorem, the quantity $E\{k'K^{-1}\underline{Z}-g(\underline{Z})|\hat{a}\}$ which is a function of $\hat{a}$ and does not depend on a, is a better estimator of $\emptyset'a$ than $\emptyset'\hat{a}$. Or, in other words, $\emptyset'\hat{a}$ is not an admissible estimator of $\emptyset'a$.

But this is a contradiction because $\hat{a} \sim N(a,G^{-1})$ and therefore it is elementary to see that $\emptyset'\hat{a}$ is admissible for $\emptyset'a$ among the class of estimators function of $\hat{a}$. (See also Cohen (1965).)

Theorem 2.3: $\hat{Z}$ is the uniformly minimum variance unbiased predictor of Z.

Proof: From lemma 2.2 we see that it is sufficient to show that the term $E\{E(Z|\underline{Z})-\hat{Z}\}^2$ is uniformly minimum in a, among unbiased predictors of Z.

An unbiased predictor $g(\underline{Z})$ of Z must satisfy $Eg(\underline{Z}) = EZ = E\{E(Z|\underline{Z})\}$; then $E\{f'a+k'K^{-1}[\underline{Z}-F'a] - g(\underline{Z})\} = 0$. Therefore it is such that $k'K^{-1}\underline{Z}-g(\underline{Z})$ is a unbiased estimator of $\emptyset'a$.

By the generalized version of Cramer-Rao inequality any

unbiased estimator of $\emptyset'a$ has its variance bounded from below by $\emptyset' I(a)^{-1}\emptyset$ where $I(a)$ is the Fisher information matrix of $\underline{Z}$ on a. It turns out that $I(a) = G$. Hence the Cramer-Rao lower bound is $\emptyset' G^{-1}\emptyset$. This is attained by $\emptyset'\hat{a}$, because $E\,\emptyset'\hat{a} = \emptyset' a$, and $E\{\emptyset'\hat{a} - \emptyset' a\}^2 = \emptyset' \mathrm{Cov}(\hat{a})\emptyset = \emptyset' G^{-1}\emptyset$.

In conclusion for any unbiased predictor $g(\underline{Z})$ of Z we have $E\{E(Z|\underline{Z}) - g(\underline{Z})\}^2 = E\{k'K^{-1}\underline{Z} - g(\underline{Z}) - \emptyset' a\}^2 \geq \emptyset' G^{-1}\emptyset = E(\emptyset'\hat{a} - \emptyset' a)^2 = E\{E(Z|\underline{Z}) - \hat{Z}\}^2$ for all a.

3. A Stein like predictor for predicting simultaneously several random variables:

Suppose now that we want to predict N random variables $Z_{n+1}, Z_{n+2}, \ldots, Z_{n+N}$ from the observations of $Z_1, Z_2, \ldots Z_n$. The assumptions that we make here are

$$\underline{Z} \sim N(F'a, K)$$

$$Z_{n+i} \sim N(f_i'a, \sigma_i^2) \qquad i = 1,2,\ldots,N$$

$$\mathrm{Cov}(\underline{Z}, Z_{n+i}) = k_i \qquad i = 1,2,\ldots,N$$

and all the Z_i's (the observations and the values to be predicted) are jointly normal. As before all the parameters appearing in the distributions are specified, except for the free vector-parameter a .

The object of this section is to exhibit a predictor $\tilde{Z}$ of the type introduced by James and Stein (1961) to estimate the mean of a multivariate normal random vector, such that

$$\sum_{i=1}^{N} E(\tilde{Z}_{n+i} - Z_{n+i})^2 < \sum_{i=1}^{N} E(\hat{Z}_{n+i} - Z_{n+i})^2$$

for all values of a .

In Section 2 we saw that the admissibility of $\hat{Z}$ ultimately reduced to the admissibility of $\emptyset'\hat{a}$ to estimate $\emptyset'a$ when $\hat{a} \sim N(a, G^{-1})$. So it is natural that in the present section

the key result will be the inadmissibility of $\Phi\hat{a}$ to estimate Φa where Φ is a $N\times p$ matrix satisfying certain conditions. This is stated in a general form in the following theorem.

<u>Theorem 3.1:</u> Consider $X \sim N(\theta, I_p)$, a p-dimensional normal random vector; let C be an $N\times p$ matrix then $\exists \eta>0$ such that for all $\theta \in R^p$

$$E\| CX\left(1-\frac{\eta}{\|X\|^2}\right) - C\theta\|^2 < E\| CX - C\theta\|^2 \qquad 3.1$$

if and only if

$$\text{max eigenvalue of } CC' < \frac{1}{2} \text{ tr } CC' \qquad 3.2$$

<u>Remark:</u> Condition (2) implies rank $C \geq 2$. In particular if C is the identity, condition (2) is satisfied if and only if $p \geq 3$, which is a classical fact in Stein-estimation (see James and Stein (1961)).

Theorem 3.1 will be proved after the following two lemmas.

<u>Lemma 3.1:</u> If $X \sim N(\theta, I_p)$, for any row vector C and any function g such that the following expectations exist, we have

$$E(cXg(\|X\|^2)) = c\theta Eg(X^2_{p+2K+2}) \qquad 3.3$$

and also

$$E\{XX'g(\|X\|^2)\} = I_p Eg(\chi^2_{p+2K+2}) + \theta\theta' Eg(\chi^2_{p+2K+4}) \qquad 3.4$$

where $K \sim \text{Poisson}\left(\frac{\|\theta\|^2}{2}\right)$.

For a proof the reader is referred to Stein (1966) where the essential technique is shown in order to prove formula 3.3; the same technique can be used to prove formula 3.4.

<u>Lemma 3.2:</u> Under the condition of theorem 3.1, we have

$$E\left\|CX\left(1-\frac{\eta}{\|X\|^2}\right) - C\theta\right\|^2 = \operatorname{tr} CC'\left[1-2\eta E\,\frac{1}{p+2K} + \eta^2 E\,\frac{1}{(p+2K)(p-2+2K)}\right] + \frac{\|C\theta\|^2}{\|\theta\|^2}(4\eta+\eta^2)E\,\frac{2K}{(p+2K)(p-2+2K)} \qquad 3.5$$

where $K \sim \text{Poisson}\left(\frac{\|\theta\|^2}{2}\right)$.

<u>Proof of Lemma 3.2:</u> We start from

$$E\left\|CX\left(1-\frac{\eta}{\|X\|^2}\right) - C\theta\right\|^2 = E\left\|C(X-\theta) - \eta\,\frac{CX}{\|X\|^2}\right\|^2$$

$$= E(X-\theta)'\,C'C(X-\theta) - 2\,E(X-\theta)'\,C'C\,\frac{X\eta}{\|X\|^2} + \eta^2\,E\,\frac{X'C'CX}{\|X\|^4}. \qquad 3.6$$

Since for two vectors in $\mathbb{R}^p$ $x'y = \operatorname{tr} yx'$, expression (3.6) can be rewritten

$$\operatorname{tr} C\, E(X-\theta)(X-\theta)'\, C' - 2\eta \operatorname{tr} C\, E \frac{X(X-\theta)'}{\|X\|^2} C' + \eta^2 \operatorname{tr} C\, E \frac{XX'}{\|X\|^4} C' \qquad 3.7$$

By Lemma 3.1 and using $E \frac{1}{\chi_n^2} = \frac{1}{n-2}$ and $E \frac{1}{\chi_n^2}^2 = \frac{1}{(n-2)(n-4)}$, expression 3.7 is equal to

$$\operatorname{tr} CC' - 2\eta \operatorname{tr} C\left\{I_p\, E \frac{1}{\chi^2_{p+2K+2}} + \theta\theta'\, E \frac{1}{\chi^2_{p+2K+4}} - \theta\theta'\, E \frac{1}{\chi^2_{p+2K+2}}\right\} C' +$$

$$\eta^2 \operatorname{tr} C\left\{I_p\, E\left[\frac{1}{\chi^2_{p+2K+2}}\right]^2 + \theta\theta'\, E\left[\frac{1}{\chi^2_{p+2K+4}}\right]^2\right\} C'$$

$$= \operatorname{tr} CC' - 2\eta \operatorname{tr} CC'\, E \frac{1}{p+2K} - 2\eta \|C\theta\|^2\, E\left\{\frac{1}{p+2K+2} - \frac{1}{p+2K}\right\} +$$

$$\eta^2 \operatorname{tr} CC'\, E \frac{1}{(p+2K)(p+2K-2)} + \eta^2 \|C\theta\|^2\, E \frac{1}{(p+2K+2)(p+2K)}$$

$$= \operatorname{tr} CC'\left[1 - 2\eta\, E \frac{1}{p+2K} + \eta^2\, E \frac{1}{(p+2K)(p+2K-2)}\right] +$$

$$\|C\theta\|^2 (4\eta + \eta^2)\, E \frac{1}{(p+2K+2)(p+2K)} .$$

Finally, to get expression 3.5 given in the statement of

Lemma 3.2 we have to show

$$E\,\frac{1}{(p+2K+2)(p+2K)} = \frac{1}{\|\theta\|^2}\,E\,\frac{2K}{(p+2K)(p+2K-2)}\ .$$

This is done as follows:

$$E\,\frac{1}{(p+2K+2)(p+2K)} = \sum_{k=0}^{\infty} e^{-\|\theta\|^2/2}\,\frac{\left(\|\theta\|^2/2\right)^k}{k!}\,\frac{1}{(p+2k+2)(p+2k)}$$

$$= \frac{2}{\|\theta\|^2}\sum_{k=0}^{\infty} e^{-\|\theta\|^2/2}\,\frac{\left(\|\theta\|^2/2\right)^{k+1}}{(k+1)!}\,\frac{k+1}{(p+2(k+1))(p+2(k+1)-2)}$$

$$= \frac{2}{\|\theta\|^2}\sum_{k=1}^{\infty} e^{-\|\theta\|^2/2}\,\frac{\left(\|\theta\|^2/2\right)^{k}}{k!}\,\frac{k}{(p+2k)(p+2k-2)}$$

$$= \frac{1}{\|\theta\|^2}\,E\,\frac{2K}{(p+2K)(p+2K-2)}\ ,$$

which completes the proof of Lemma 3.2. Now we can turn to the proof of Theorem 3.1.

<u>Proof of Theorem 3.1:</u> The key to the proof is to observe that

$$\max_{\theta}\frac{\|C\theta\|^2}{\|\theta\|^2} = \text{max eigenvalue of } CC'\ .$$

First if

$$\text{max eigenvalue of } CC' \leq \left(\frac{1-\varepsilon}{2}\right) \text{tr } CC' \,, \qquad 3.8$$

then $E\|CX\left(1 - \frac{\eta}{\|X\|^2}\right) - C\theta\|^2$ is bounded by

$$\text{tr } CC' \Bigg\{ 1 - 2\eta \, E \frac{1}{p+2K} + \eta^2 \, E \frac{1}{(p+2K)(p-2+2K)} +$$

$$2(1-\varepsilon)\eta \, E \frac{2K}{(p+2K)(p-2+2K)} + (1-\varepsilon)\eta^2 \, E \frac{K}{(p+2K)(p-2+2K)} \Bigg\} \,. \qquad 3.9$$

In turn to bound expression 3.9 we need $p \geq 3$; but, as observed in the remark on page 12, this is implied by 3.8. Then expression 3.9 is bounded by

$$\text{tr } CC' \left\{ 1 - 2\varepsilon\eta \, E \frac{1}{p+2K} + \eta^2 \, E \frac{1}{p+2K} \right\} .$$

Therefore if we pick $\eta = \varepsilon$, we get

$$E\|CX\left(1 - \frac{\varepsilon}{\|X\|^2}\right) - C\theta\|^2 \leq \text{tr } CC' \left(1 - \varepsilon^2 \, E \frac{1}{p+2K}\right) < \text{tr } CC' = E\|CX - C\theta\|^2 \,.$$

Conversely if max eigenvalue of $CC' \geq \frac{1}{2} \text{ tr } CC'$ we can choose the direction of θ such that

$$\frac{\|C\theta\|^2}{\|\theta\|^2} = \text{max eigenvalue of } CC'$$

and therefore such that

$$E\left\|CX\left(1-\frac{\eta}{\|X\|^2}\right)-C\theta\right\|^2 \geq \operatorname{tr} CC'\left[1-2\eta\, E\,\frac{1}{p+2K}+\right.$$

$$\left.2\eta\, E\,\frac{2K}{(p+2K)(p-2+2K)}+\eta^2\, E\,\frac{K+1}{(p+2K)(p-2+2K)}\right]$$

$$=\operatorname{tr} CC'\left[1-2\eta\, E\,\frac{p-2}{(p+2K)(p-2+2K)}+\eta^2\, E\,\frac{K+1}{(p+2K)(p-2+2K)}\right].$$

Now, for any $\eta > 0$, there exists θ large enough such that the above quantity is strictly greater than $\operatorname{tr} CC'$, because when $\|\theta\| \to +\infty$

$$E\,\frac{p-2}{(p+2K)(p-2+2K)} = o\left(E\,\frac{K+1}{(p+2K)(p-2+2K)}\right).$$

This completes the proof of Theorem 3.1.

<u>Application of Theorem 3.1 to the prediction of Z_{n+1}, $Z_{n+2},\ldots,Z_{n+N}$ using $Z_1, Z_2,\ldots,Z_n$:</u>

Parallel to the notation $\emptyset = FK^{-1}k-f$, let us define $\emptyset_i = FK^{-1}k_i-f_i \quad i=1,2,\ldots,N$.

From the results of Section 2, we know that the individual best linear unbiased predictors of each Z_{n+i}, $i=1,2,\ldots,N$, based on $\underline{Z}$, are

$$\hat{z}_{n+i} = f_i'\hat{a} + k_i'K^{-1}[\underline{Z}-F'\hat{a}]$$

$$= k_i'K^{-1}\underline{Z} - \emptyset_i'\hat{a} \qquad i=1,2,\ldots,N$$

And we know that they are individually admissible. The fact that it is not the case, in general, when they are used simultaneously, is the object of the following theorem:

<u>Theorem 3.2</u>: For $i=1,2,\ldots,N$, define

$$\tilde{z}_{n+i} = k_i' K^{-1}\underline{Z} - \emptyset_i' \hat{a}\left(1-\frac{\eta}{\hat{a}'G\hat{a}}\right) \qquad 3.10$$

then $\exists\eta > 0$ such that, for all a

$$\sum_{i=1}^{N} E(\tilde{z}_{n+i} - z_{n+i})^2 < \sum_{i=1}^{N} E(\hat{z}_{n+i} - z_{n+i})^2 \qquad 3.11$$

if and only if

$$\text{max eigenvalue of } [\emptyset_i'G^{-1}\emptyset_j] < \sum_{i=1}^{N} \emptyset_i'G^{-1}\emptyset_i \qquad 3.12$$

where $[\emptyset_i'G^{-1}\emptyset_j]$ is the $N\times N$ matrix whose (i,j) element is $\emptyset_i'G^{-1}\emptyset_j$.

<u>Proof</u>: Since $\underline{Z} \sim N(F'a,K)$ we have $K^{-\frac{1}{2}}\underline{Z} \sim N(K^{-\frac{1}{2}} F'a, I_p)$.

Consider an orthogonal matrix $H=\begin{pmatrix} H_1 \\ H_2 \end{pmatrix}$ such that

$v(H_1') = v(K^{-\frac{1}{2}}F')$ where $v(H_1')$ stands for the vector space generated by the columns of H_1'. Then

$$HK^{-\frac{1}{2}}\underline{Z} \sim N\left(\begin{matrix} H_1K^{-\frac{1}{2}}F'a \\ 0 \end{matrix}, I_p\right) .$$

let $M = H_1K^{-\frac{1}{2}}F'$; it is of size $p\times p$ and non singular since we assumed that $FK^{-1}F'$ is of full rank. Let $\alpha = Ma$ and $\hat{\alpha} = M\hat{\alpha}$, then $\hat{\alpha} \sim N(M\hat{a}, MG^{-1}M')$. Let us show that $MG^{-1}M'$ is actually I_p : we start from

$$\begin{aligned} M'M &= FK^{-\frac{1}{2}}H_1'H_1K^{-\frac{1}{2}}F' \\ &= FK^{-\frac{1}{2}}(I-H_2'H_2)K^{-\frac{1}{2}}F' \\ &= FK^{-\frac{1}{2}}F' - FK^{-\frac{1}{2}}H_2'H_2K^{-\frac{1}{2}}F' \end{aligned}$$

But $H_2K^{-\frac{1}{2}}F' = 0$; therefore $M'M = G$. Then $G^{-\frac{1}{2}}M'MG^{-\frac{1}{2}} = I_p$. This means that $MG^{-\frac{1}{2}}$ is orthogonal, hence $MG^{-1}M' = I_p$. In conclusion, we have $\hat{\alpha} \sim N(\alpha, I_p)$.

From lemma 2.2 we can write

$$\sum_{i=1}^{N} E(\tilde{Z}_{n+i} - Z_{n+i})^2 = \sum_{i=1}^{N} E(Z_{n+i} - E(Z_{n+i}|\underline{Z}))^2 + \sum_{i=1}^{N} E(\tilde{Z}_{n+i} - E(Z_{n+i}|\underline{Z}))^2 \qquad 3.13$$

the first term of the right hand side of 3.13 is $\sum_{i=1}^{N} (\sigma_i^2 - k_i' K^{-1} k_i)$. On the other hand, since

$E(Z_{n+i}|\underline{Z}) = k_i' K^{-1}\underline{Z} - \emptyset_i' a$ the second term of the right hand side of 3.13 can be rewritten

$$\sum_{i=1}^{N} E\left(\emptyset_i'\hat{a}\left(1 - \frac{\eta}{\hat{a}'G\hat{a}}\right) - \emptyset_i' a\right)^2 \qquad 3.14$$

Note that $||\hat{\alpha}^2|| = \hat{\alpha}'\hat{\alpha} = \hat{\alpha}'M'M\hat{\alpha} = \hat{a}'G\hat{a}$; and let C be the $N\times p$ matrix whose i^{th} row is $\emptyset_i' M$. Then expression 3.14 becomes

$$\sum_{i=1}^{N} E\left(\emptyset_i' M\hat{\alpha}\left(1 - \frac{\eta}{||\hat{\alpha}||^2}\right) - \emptyset_i' M\alpha\right)^2 = E\left|\left|C\hat{\alpha}\left(1 - \frac{\eta}{||\hat{\alpha}||^2}\right) - C\alpha\right|\right|^2 .$$

Since $\hat{\alpha} \sim N(\alpha, I_p)$, by Theorem 3.1 we know that $\exists \eta > 0$ such that for all α

$$E\left|\left|C\hat{\alpha}\left(1 - \frac{\eta}{||\hat{\alpha}||^2}\right) - C\alpha\right|\right|^2 < E||C\hat{\alpha} - C\alpha||^2$$

if and only if maxeigenvalue of $CC' < \frac{1}{2}\operatorname{tr} CC'$.

To finish the proof let us observe on the one hand that $CC' = [\emptyset_i' G^{-1}\emptyset_j]$, and on the other hand (by going backward in the computation) that

$$E||C\hat{\alpha} - C\alpha||^2 = \sum_{i=1}^{N} E\{E(Z_{n+i}|\underline{Z}) - \hat{Z}_{n+i}\}^2$$

this, after another application of lemma 2.2, completes the proof of Theorem 3.2.

4. A non linear predictor of a single random variable Z, based on $Z_1, Z_2, \ldots Z_n$.

Coming back to the problem of predicting a single Z from the observations $\underline{Z}$, we show in this section another way to reduce the extra-term $\emptyset' G^{-1} \emptyset$, in the mean squared error of the estimator $\hat{Z}$, that we have already discussed in Section 2.

The idea is to try to dispense with unbiasedness. This leads to a predictor $\hat{Z}_a$, which depends on the unspecified vector parameter a. It is therefore of no use itself but the predictor denoted symbolically $\hat{Z}_{\hat{a}}$, obtained by substituting $\hat{a}$ for a in $\hat{Z}_a$, turns out to be interesting; we will denote it Z^*.

Preliminary calculations show that the predictor $\hat{Z}_a = \lambda_1 Z_1 + \ldots + \lambda_n Z_n$ which minimizes $E(\hat{Z}_a - Z)^2$, with no unbiasedness restriction with respect to a, is

$$\hat{Z}_a = k' K^{-1} \underline{Z} - \frac{\emptyset' a}{1 + a' G a} \, a' F K^{-1} \underline{Z} \qquad 4.1$$

and its risk is

$$E(\hat{Z}_a - Z)^2 = \sigma^2 - k' K^{-1} k + \frac{(\emptyset' a)^2}{1 + a' G a} \qquad 4.2$$

Note that $\sup\limits_a \frac{(\emptyset' a)^2}{1 + a' G a} = \emptyset' G^{-1} \emptyset$ which is the third term in

the risk of $\hat{Z}$.

So the predictor we want to study in this section is

$$Z^* = k'K^{-1}\underline{Z} - \frac{\emptyset'\hat{a}}{1+\hat{a}'G\hat{a}} \cdot \hat{a}'FK^{-1}\underline{Z} \qquad 4.3$$

as derived from formula 4.1 by substitution of $\hat{a}$ for a .

In the sequel we assume that Z and $\underline{Z}$ are jointly normally distributed.

<u>Theorem 4.1</u>: The predictor Z^* can be reexpressed as

$$Z^* = \hat{Z} + \frac{\emptyset'\hat{a}}{1+\hat{a}'G\hat{a}} \qquad 4.4$$

and its risk is

$$E(Z^*-Z)^2 = \sigma^2 - k'K^{-1}k + \mathrm{Var}\left(\frac{\emptyset'\hat{a}\,\hat{a}'G\hat{a}}{1+\hat{a}'G\hat{a}}\right) + \left\{E\left(\frac{\emptyset'\hat{a}}{1+\hat{a}'G\hat{a}}\right)\right\}^2 \qquad 4.5$$

To prove Theorem 4.1 we need two lemmas.

<u>Lemma 4.1</u>: Consider $X \sim N(\mu,\Sigma)$ of size $n\times 1$; suppose Σ is positive definite. Let M be a $p\times n$ matrix $(p \leq n)$ of full rank, and ν a $p\times 1$ vector. Then

$$E(X|MX=\nu) = \mu - \Sigma M'(M\Sigma M')^{-1}M\mu + \Sigma M'(M\Sigma M')^{-1}\nu$$

$$\mathrm{Cov}(X|MX=\nu) = \Sigma(I - M'(M\Sigma M')^{-1}M\Sigma)$$

For a proof of Lemma 4.1 the reader is referred to Cabannes (1979).

Lemma 4.2: $E(\underline{Z}|\hat{a}) = F'\hat{a}$ and $E(Z|\hat{a}) = -\emptyset'a + k'K^{-1}F'\hat{a}$

Lemma 4.2 can be proved as an application of Lemma 4.1. Again we skip the calculations.

Proof of Theorem 4.1: To prove 4.4 we write

$$Z^* - \frac{\emptyset'\hat{a}}{1+\hat{a}'G\hat{a}} = k'K^{-1}\underline{Z} - \frac{\emptyset'\hat{a}\,\hat{a}'FK^{-1}\underline{Z}}{1+\hat{a}'G\,\hat{a}} - \frac{\emptyset'\hat{a}}{1+\hat{a}'G\,\hat{a}}$$

$$= k'K^{-1}\underline{Z} - \frac{\emptyset'\hat{a}\,\hat{a}'G\,\hat{a}}{1+\hat{a}'G\,\hat{a}} - \frac{\emptyset'\hat{a}}{1+\hat{a}'G\,\hat{a}} = k'K^{-1}\underline{Z} - \emptyset'\hat{a} = \hat{Z}$$

Hence $Z^* = \hat{Z} + \dfrac{\emptyset'\hat{a}}{1+\hat{a}'G\,\hat{a}}$

Next the risk of Z^* is

$$E(Z^*-Z)^2 = E\left(\hat{Z}-Z + \frac{\emptyset'\hat{a}}{1+\hat{a}'G\,\hat{a}}\right)^2$$

$$= E(\hat{Z}-Z)^2 + E\left[\left(\frac{\emptyset'\hat{a}}{1+\hat{a}'G\,\hat{a}}\right)^2\right] +$$

$$2E\left[(\hat{Z}-Z)\left(\frac{\emptyset'\hat{a}}{1+\hat{a}'G\,\hat{a}}\right)\right] \qquad 4.6$$

To compute the cross-product term in 4.6 we condition on $\hat{a}$:

$$E\left[(\hat{Z}-Z)\left(\frac{\emptyset'\hat{a}}{1+\hat{a}'G\,\hat{a}}\right)|\hat{a}\right] = \frac{\emptyset'\hat{a}}{1+\hat{a}'G\,\hat{a}}\;E(\hat{Z}-Z|\hat{a})$$

and from Lemma 4.2 we have

$$E(\hat{Z}-Z\,|\,\hat{a}) = \lambda' E(\underline{Z}\,|\,\hat{a}) - E(Z\,|\,\hat{a})$$

$$= (k'K^{-1} - \emptyset' G^{-1} F K^{-1}) F'\hat{a} - (k'K^{-1}F'a - \emptyset'\hat{a})$$

$$= \emptyset'(a-\hat{a})$$

Therefore

$$E\left[(\hat{Z}-Z)\left(\frac{\emptyset'\hat{a}}{1+\hat{a}'G\,\hat{a}}\right)\right] = E\left[\emptyset'(a-\hat{a})\ \frac{\emptyset'\hat{a}}{1+\hat{a}'G\,\hat{a}}\right]$$

$$= \emptyset' a\ E\left(\frac{\emptyset'\hat{a}}{1+\hat{a}'G\,\hat{a}}\right) - E\left[\frac{(\emptyset'\hat{a})^2}{1+\hat{a}'G\,\hat{a}}\right]$$

$$= -\,\mathrm{Cov}\left(\emptyset'\hat{a}\ ,\ \frac{\emptyset'\hat{a}}{1+\hat{a}'G\,\hat{a}}\right)$$

Then

$$E(Z^*-Z)^2 = \sigma^2 - k'K^{-1}k + \emptyset' G^{-1}\emptyset + E\left[\left(\frac{\emptyset'\hat{a}}{1+\hat{a}'G\,\hat{a}}\right)^2\right] -$$

$$2\,\mathrm{Cov}\left(\emptyset'\hat{a}\ ,\ \frac{\emptyset'\hat{a}}{1+\hat{a}\,G\,\hat{a}}\right)$$

Formula 4.5 follows after some more manipulation, noting that $\emptyset' G^{-1}\emptyset = \mathrm{Var}\,(\emptyset'\hat{a})$. ■

The next problem is to compare the risks $R(a,Z^*) = E(Z^*-Z)^2$ and $R(a,\hat{Z}) = E(\hat{Z}-Z)^2$. Let $R(\hat{Z}) \triangleq R(a,\hat{Z})$ because it does not depend on a. Since we showed in Section 2 the admissibility of $\hat{Z}$, Z^* cannot be uniformly better than $\hat{Z}$ when a varies.

However, we have the following result

<u>Theorem 4.2</u>: $R(0,Z^*) < R(\hat{Z})$ and $\lim_{\|a\| \to +\infty} R(a,Z^*) = R(\hat{Z})$

<u>Proof</u>: When $a = 0$, we have $E\left(\frac{\emptyset'\hat{a}}{1+\hat{a}'G\hat{a}}\right) = 0$ because the distribution of $\hat{a}$ then is $N(0,G^{-1})$ and $\frac{\emptyset'\hat{a}}{1+\hat{a}'G\hat{a}}$ has a distribution symmetric about zero. Therefore $R(0,Z^*) = \sigma^2 - k'K^{-1}k + \mathrm{Var}\left(\emptyset'\hat{a}\ \frac{\hat{a}'G\hat{a}}{1+\hat{a}'G\hat{a}}\right)$ and again since $\hat{a} \sim N(0,G^{-1})$ we have $\mathrm{Var}\left(\emptyset'\hat{a}\ .\ \frac{\hat{a}'G\hat{a}}{1+\hat{a}'G\hat{a}}\right) < \mathrm{Var}(\emptyset'\hat{a}) = \emptyset'G^{-1}\emptyset$ hence $R(0,Z^*) < R(\hat{Z})$.

Next note that when $\|a\| \to +\infty$ the term $\frac{\emptyset'\hat{a}}{1+\hat{a}'G\hat{a}}$ tends to zero in probability, and therefore also in distribution. And since there exists a constant c such that $\forall b \in \mathbb{R}^p$, $\left|\frac{\emptyset'b}{1+b'Gb}\right| < c$ we deduce by a classical convergence theorem that all the moments of $\frac{\emptyset'\hat{a}}{1+\hat{a}'G\hat{a}}$ tend to zero. Then because $\mathrm{Var}\,\emptyset'\hat{a} = \emptyset'G^{-1}\emptyset$ we have

$$\lim_{\|a\| \to +\infty} \mathrm{Var}\left(\emptyset'\hat{a} - \frac{\emptyset'\hat{a}}{1+\hat{a}'G\hat{a}}\right) + E\left[\left(\frac{\emptyset'\hat{a}}{1+\hat{a}'G\hat{a}}\right)^2\right] = \emptyset'G^{-1}\emptyset$$

This completes the proof of Theorem 4.2. ■

We state briefly some final results without proving them, referring the interested reader to the report of the author (1979).

The risk of Z^* can be reexpressed as follows

$R(a,Z^*) = R(\hat{Z}) + \xi(a)$ where

$$\xi(a) = \tfrac{1}{2}\, \emptyset' G^{-1} \emptyset \;\; E\left[\frac{1}{1+\chi^2_{p+2K}} - E\,\frac{1}{1+\chi^2_{p+2K+2}}\right] +$$

$$\tfrac{5}{2}(\emptyset' a)^2 \left[E\,\frac{1}{1+\chi^2_{p+2K+2}} - E\,\frac{1}{1+\chi^2_{p+2K+4}}\right]$$

and $K \sim \text{Poisson}\left(\frac{a'Ga}{2}\right)$. And this, combined with the following approximation (Stein 1966)

$$E\,\frac{1}{\chi^2_{p+2K}} \approx \frac{1}{p-2+t}\left\{1 - \frac{2t}{(p-2+t)^2}\right\}$$

where $t = a'Ga$, can be used to compute approximate values of the risk function of Z^*.

<u>Illustration of the preceding method in the estimation of the mean of i.i.d. normal random variables with known variance</u>:

Suppose that $Z, Z_1, Z_2, \ldots Z_n$ are i.i.d. $N(m,\sigma^2)$ then of course the predictors $\hat{Z}$ and Z^* truly estimate the mean m, so let's denote them $\hat{m}$ and m^*. Note that

$$E(\hat{m}-m)^2 = E(\hat{m}-Z)^2 - \sigma^2$$

and $$E(m^*-m)^2 = E(m^*-Z)^2 - \sigma^2$$

let $$R(m,\hat{m}) = E(\hat{m}-m)^2 \text{ and}$$

$$R(m,m^*) = E(m^*-m)^2$$

then if we define $\xi_0(m)$ by

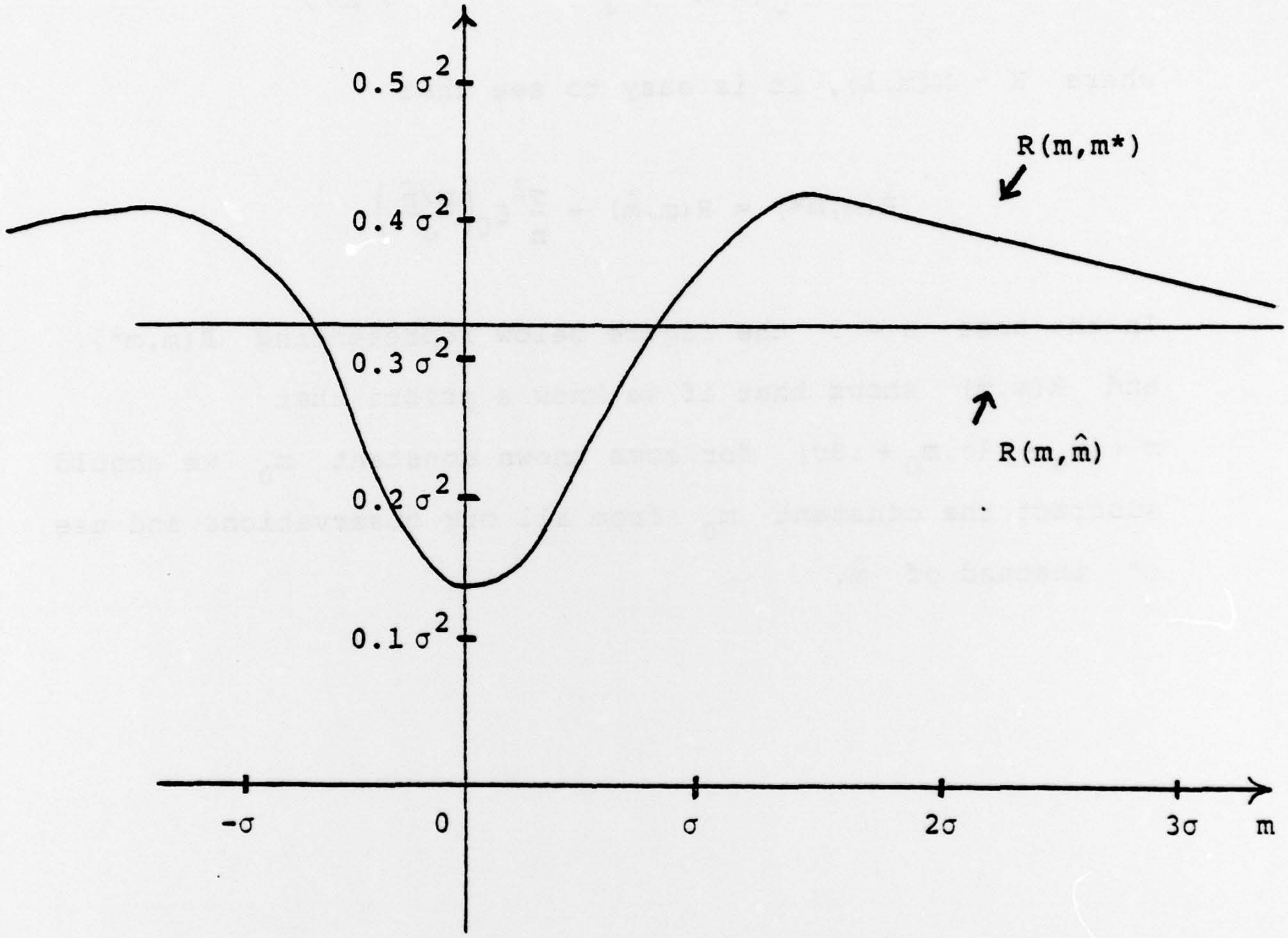
$$\xi_0(m) = E\left[\left(\frac{X}{1+X^2}\right)^2\right] - 2\,\mathrm{cov}\left(X, \frac{X}{1+X^2}\right)$$

where $X \sim N(m,1)$, it is easy to see that

$$R(m,m^*) = R(m,\hat{m}) + \frac{\sigma^2}{n}\xi_0\left(\frac{m\sqrt{n}}{\sigma}\right)$$

In the case $n = 3$ the figure below representing $R(m,m^*)$ and $R(m,\hat{m})$ shows that if we know a priori that $m \in [m_0 - .8\sigma, m_0 + .8\sigma]$ for some known constant m_0 we should subtract the constant m_0 from all our observations and use m^* instead of $\hat{m}$.

(see the figure next page)



<u>Figure</u>: Comparison of the risk functions of $\hat{m}$ and m*.

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an element of $\mathbb{R}$-squared

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The variation of temperature or of pollutant concentrations over a geographic area are adequately represented by random fields. Given a real-valued random field $\{Z(x), x \in \mathbb{R}^2\}$ a basic problem is to interpolate Z over an area A from measurements taken at n stations $x_1, x_2, \ldots, x_n$, when the distribution of Z is only partially specified. This is the motivation of the present paper,

It is shown that if the joint distributions are Gaussian the best linear unbiased predictor (B.L.U.E.) is (among other properties) admissible when used to predict Z at a single point, but inadmissible in general when used to predict the values of the field at several points. A Stein-like predictor is produced which is uniformly better than the B.L.U.E. in the latter case. A non-linear predictor, based on relaxing the unbiasedness condition on the B.L.U.E., is also proposed and shown to be in some cases preferable.

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